MS3L_12778

XXI International Congress of Theoretical and Applied Mechanics
Warsaw, Poland, August 15–21, 2004

Nano-scale Planar Field Projection of Atomistic Decohesion of Crystalline Solids

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An atomistic cohesive zone of a crack tip is characterized by a nano-scale planar field projection of the elastic field of a crack tip, analyzing the near-tip deformation field with a molecular statics simulation of gold. The atomistic simulation with an embedded atom method (EAM) potential is made for a crystal decohesion along $[11\bar{2}]$ direction in a (111) plane. A general form of planar elastic field projection is derived to identify cohesive-zone constitutive relations from the elastic field of a cohesive crack tip sitting on an interface between two anisotropic solids. The cohesive traction, the interface separation and the surface-stress gradient caused by gradual variation of surface formation within the cohesive zone can be obtained by the nano-scale planar field projection. Details of energy partition in various modes of nano-scale separation processes are analyzed with atomistic simulations and the field projection method.

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